①

ON APPROXIMATE EXPRESSIONS FOR THE EXPONENTIAL
INTEGRAL AND THE ERROR FUNCTION

Richard Bellman

P - 175
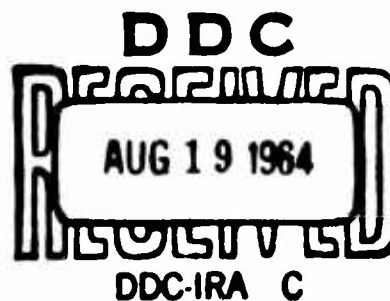
19 September 1950

Approved for OTS release

DDC

AUG 19 1964

DDC-IRA C

ON APPROXIMATE EXPRESSIONS FOR THE EXPONENTIAL INTEGRAL AND THE ERROR FUNCTION

Richard Bellman

§1. Introduction.

In many important applications of mathematical physics, the final numerical answer depends upon the evaluation of a Laplace transform

$$(1) \qquad g(y) = \int_0^\infty e^{-xy} f(x) dx, \qquad Re(y) > 0.$$

Integrating by parts n times, the result is

$$(2) \qquad g(y) = \frac{f(0)}{y} + \frac{f^1(0)}{y^2} + \cdots + \frac{f^{(n-1)}(0)}{y^n} + \frac{1}{y^n} \int_0^\infty e^{-xy} f^{(n)}(x) dx.$$

If $f(0) \neq 0$, we may use the first n terms as an approximation to $g(y)$. The error term is the integral on the right-hand side of (2) which is bounded by

$$(3) \qquad y^{-(n+1)} \max_{0 \leq x < \infty} |f^{(n)}(x)|$$

for y real and by

$$(4) \qquad |y|^{-n} \max_{0 \leq x < \infty} |f^{(n)}(x)| \,/\, Re(y),$$

in case y is complex. In many cases of importance, the series

$$(5) \qquad S(y) = \sum_{k=0}^\infty f^{(k)}(0) \,/\, y^{k+1}$$

is divergent for all y. Consequently, in order to make maximum use of (2), n must be chosen as a function of y to minimize the expressions in (3) or (4). The fact that $S(y)$ is a divergent asymptotic series as $y \rightarrow \infty$ imposes a lower bound on the magnitude of the error term.

The question arises then as to whether it is possible to obtain a better approximation to $g(y)$ than that given by (2) using some rational function of $1/y$, with coefficients determined by the $f^{(k)}(0)$. One way of obtaining those rational approximations is that of expanding $S(y)$ into a formal continued fraction and using the n-th convergents.

The purpose of the present note is to indicate another method which under all circumstances yields an error term less than or equal to that given by (3) or (4), and in general may be expected to improve it considerably. After indicating the general method, we apply it to the two most commonly encountered non-elementary transcendents

$$(6) \qquad E_1(y) = \int_y^\infty \frac{e^{-x}}{x} \, dx = e^{-y} \int_0^\infty \frac{e^{-xy}}{1+x} \, dx$$

$$1 - \mathrm{Erf}(y) = \frac{1}{\sqrt{2\pi}} \int_y^\infty e^{-x^2} dx = \frac{e^{-\sqrt{y}} \, e^{-1/4}}{\sqrt{2\pi}} \int_0^\infty \frac{e^{-x\sqrt{y}}}{(1+x)^{1/2}} \, dx \, .$$

The following result is obtained:

<u>Theorem</u>: <u>If</u> $y > 0$, <u>there</u> <u>exist for</u> <u>each</u> $n \geq 1$, <u>polynomials in</u> $\frac{1}{y}$, $Q_n(y)$, $R(y)$ <u>with</u> <u>the properties that</u>

$$(7) \qquad \left| \int_0^\infty \frac{e^{-xy}}{1+x} \, dx - \frac{R_n(y)}{Q_n(y)} \right| \leq \frac{n!}{2^{2n+1} \, y^{n+1} \, Q_n(y)} < \frac{n!}{2^{2n+1} \, y^{n+1}} \, ,$$

where

(8) (a) $\qquad Q_n(y) = 1 + \displaystyle\sum_{i=1}^{n} a_i y^{-i}$,

(b) $\qquad a_k = n! \dfrac{2^{n-k+1}}{\left[(n+1-k)!\right]^2} \displaystyle\prod_{\ell=1}^{n-k+1}\left(\dfrac{(n+1)^2 - \ell^2}{2\ell + 1}\right)$,

(c) $\qquad R_n(y) = P_n(y) + \displaystyle\sum_{i=1}^{n} a_i y^{-i} P_{n-i}(y) - a_{n+1} y^{-n-1}$,

(d) $\qquad P_k(y) = \displaystyle\sum_{\ell=0}^{k-1} (-1)^\ell \, \ell! \, y^{-(\ell+1)}$, $\qquad k = 1, 2, \cdots$.

If y is complex, the right-side of (7) is replaced by

(9) $\qquad \dfrac{n!}{2^{2n+1} \, |y|^n \, |Q_n(y)| \, \mathrm{Re}(y)}$.

A similar result holds for any integral of the form

(10) $\qquad I_a(y) = \displaystyle\int_0^{\infty} \dfrac{e^{-xy}}{(1+x)^a} \, dx$.

Applied to the integral in (7), $I_1(y)$, the method discussed in (2) et seq. yields the bound $n!/y^{n+1}$. The best possible bound is obtained by taking $n = [y]$, yielding an error term approximately equal to $e^{-y}\sqrt{2\pi y}$. The best possible bound obtained from the above theorem is obtained by taking $n = 2y$ and is approximately $e^{-4y}\sqrt{2\pi y}$.

Although these functions in the cases a = 1/2 and 1 have been extensively tabulated for real y, there may still be some practical application of the inequalities we obtain, since in several important applications these functions occur with complex argument. We discuss below a device which may be employed if $Re(y)$ is small.

§2. The method.

Let us consider first the simplest case where $f(0) \neq 0$, y is real, and we will be satisfied with an approximation with an error of order $1/y^2$ as $y \rightarrow \infty$. Integrating by parts once, we obtain

$$(1) \qquad g(y) = \frac{f(0)}{y} + \frac{1}{y} \int_0^\infty e^{-xy} f^1(x) dx$$

$$= \frac{f(0)}{y} + \frac{1}{y} \int_0^\infty e^{-xy} \left[f^1(x) + af(x) + b \right] dx$$

$$- \frac{a}{y} \int_0^\infty e^{-xy} f(x) dx - \frac{b}{y^2} .$$

From this follows

$$(2) \qquad g(y) \left(1 + \frac{a}{y} \right) - \left(\frac{f(0)}{y} + \frac{b}{y^2} \right) = \frac{1}{y} \int_0^\infty e^{-xy} \left[f^1(x) + af(x) + b \right] dx , .$$

whence

$$(3) \qquad \left| g(y) \left(1 + \frac{a}{y} \right) - \left(\frac{f(0)}{y} + \frac{b}{y^2} \right) \right| \leq \underset{0 \leq x < \infty}{\text{Max}} \left| f^1(x) + af(x) + b \right| / y^2 .$$

The parameters a and b are now to be chosen so as to minimize the right-hand side. In general, this is a difficult problem, which we do not

propose to discuss here. Nevertheless, in many cases, a few trials will yield values of a and b which appreciably reduce the error term.

Let us now proceed to the general case. After n-integrations by parts, we have

$$(4) \qquad g(y) = P_n(y) + \frac{1}{y^n} \int_0^\infty e^{-xy} f^{(n)}(x)dx ,$$

where we have set

$$(5) \qquad P_n(y) = \sum_{k=0}^{n-1} f^{(k)}(0)y^{-(k+1)} , \qquad n = 1, 2, \cdots.$$

We now write $g(y)$ as follows:

$$(6) \qquad g(y) = P_n(y) + \frac{1}{y^n} \int_0^\infty e^{-xy} \left[f^{(n)}(x) + a_1 f^{(n-1)}(x) + \cdots + a_n f(x) + a_{n+1} \right] dx$$

$$- \frac{1}{y^n} \sum_{i=1}^n a_i \int_0^\infty e^{-xy} f^{(n-i)}(x)dx - \frac{a_{n+1}}{y^{n+1}} .$$

Utilizing (4) to eliminate the integrals $\int_0^\infty e^{-xy} f^{(n-i)}(x)dx$, this leads to the inequality

$$(7) \qquad \left| g(y) - \frac{R_n(y)}{Q_n(y)} \right| \leq \frac{\displaystyle\max_{0 \leq x < \infty} \left| f^{(n)}(x) + a_1 f^{(n-1)}(x) + \cdots + a_n f(x) + a_{n+1} \right|}{y^{n+1} \left| Q_n(y) \right|} ,$$

where we have set

$$(8) \qquad Q_n(y) = 1 + \sum_{i=1}^n a_i y^{-i}$$

$$R_n(y) = P_n(y) + \sum_{i=1}^n a_i y^{-i} P_{n-i}(y) - a_{n+1} y^{-n-1} .$$

The error term depends upon the polynomial $Q_n(y)$ and the functional

$$(9) \qquad c_n(f) = \min_{a_i} \max_{0 \leq x < \infty} \left| f^{(n)}(x) + a_1 f^{(n-1)}(x) + \cdots + a_n f(x) + a_{n+1} \right| .$$

We may conceive of $c_n(f)$ as a measure of the deviation of $f(x)$ from a function of the form

$$(10) \qquad h(x) = \sum_{k=1}^{N} p_k(x) e^{b_k x} ,$$

where each $p_k(x)$ is a polynomial in x.

In the succeeding section we determine $c_n(f)$ for the case where $f(x) = 1/1+x$.

§3. Application to the Exponential Integral.

Referring to (6) of §1, we see that it is sufficient to treat the Laplace transform

$$(1) \qquad g(y) = \int_0^\infty \frac{e^{-xy}}{1+x} \, dx .$$

Consequently, we wish to determine

$$(2) \qquad \min_{a_i} \max_{0 \leq x < \infty} \left| \frac{n!}{(1+x)^{n+1}} - \frac{a_1(n-1)!}{(1+x)^n} + \cdots + \frac{(-1)^n a_n}{1+x} + (-1)^n a_{n+1} \right| .$$

Upon setting $\frac{1}{1+x} = \frac{1+x'}{2}$, this reduces to

$$(3) \qquad \min_{a_i} \max_{-1 \leq x \leq 1} \left| \frac{n! \, (1+x)^{n+1}}{2^{n+1}} - \frac{(n-1)! \, a_1 (1+x)^n}{2^n} + \cdots + (-1)^n a_{n+1} \right| .$$

Since the degree of the polynomial is $(n+1)$ and the coefficient of the highest degree term is $n!/2^{n+1}$, it follows that the minimal polynomial is the $(n+1)$st Chebychev polynomial

$$(4) \qquad \frac{n! \, T_{n+1}(x)}{2^{n+1}} = \frac{n! \, \cos(n+1) \, \arccos x}{2^{2n+1}}$$

$$= \frac{n! \, (1+x)^{n+1}}{2^{n+1}} - \frac{(n-1)! \, a_1 (1+x)^n}{2^n} + \cdots + (-1)^n \, a_{n+1} \, ,$$

and that

$$(5) \qquad c_n\left(\frac{1}{1+x}\right) = n!/2^{2n+1} \, .$$

Referring to (7) of the previous section, we see that before we can apply the inequality with confidence, we must know something about the location of the roots of $Q_n(y) = 0$. Using (4), we shall determine the a_1 and show that they are all positive, whence $Q_n(y) > 1$ for $y > 0$.

For $n = 1, 2, 3$, the roots of $Q_n(y) = 0$ are all negative, and we hazard a guess that this is true in general. This result, if valid, would be of importance in applying the inequality to the case where y is complex.

Since

$$(6) \qquad T_{n+1}(x) = T_{n+1}(-1 + (1+x)) = \sum_{k=0}^{n+1} \frac{T_{n+1}^{(k)}(-1)(1+x)^k}{k!} \, ,$$

we obtain from the identity of (4),

$$(7) \qquad \frac{(-1)^{n-k+1} a_{n-k+1} \, k!}{2^{n-k+1}} = \frac{n!}{2^{n+1}} \, \frac{T_{n+1}^{(k)}(-1)}{k!} \, .$$

To determine $T_{n+1}^{(k)}(-1)$, we use the fact that $T_{n+1}(x)$ satisfies the differential equation

(8) $$(1 - x^2)T_{n+1}''(x) - xT_{n+1}'(x) + (n+1)^2 T_{n+1}(x) = 0.$$

Hence $T_{n+1}^{(k)}(x)$ satisfies the equation

(9) $$(1 - x^2)T_{n+1}^{(k+2)}(x) - (2k+1)xT_{n+1}^{(k+1)}(x) + ((n+1)^2 - k^2)T_{n+1}^{(k)}(x) = 0.$$

Thus

(10) $$T_{n+1}^{(k+1)}(-1) = - \left[\frac{(n+1)^2 - k^2}{2k+1} \right] T_{n+1}^{(k)}(-1) ,$$

whence finally

(11) $$T_{n+1}^{(k)}(-1) = (-1)^{n+k+1} \prod_{k=1}^{k} \left(\frac{(n+1)^2 - k^2}{2k+1} \right), \qquad k = 1, 2, \cdots$$

$$= (-1)^{n+1} , \qquad\qquad k = 0.$$

Substituting in (7), we obtain

(12) $$a_k = \frac{n! \, 2^{n+1-k}}{[(n+1-k)!]^2} \prod_{\ell=1}^{n+1-k} \left(\frac{(n+1)^2 - \ell^2}{2\ell+1} \right) , \qquad k \neq n+1,$$

$$= n! , \qquad\qquad k = n+1.$$

This completes the proof of the theorem stated above.

If $\text{Re}(y)$ is small, the term $1/\text{Re}(y)$ may greatly increase the error term, particularly for small n. We may overcome this to some extent by

writing

$$(13) \quad \int_0^\infty e^{-xy} f^{(n)}(x)dx = \frac{1}{y^n} \int_0^\infty \frac{e^{-xy}}{(1+x)^2} \left[\frac{(-1)^n n!}{(1+x)^{n-2}} + \frac{a_1(n-1)!}{(1+x)^{n-3}} + \cdots + (-1)^{n-1} a_{n-1} \right]$$

minus the appropriate terms.

From this we obtain as a bound

$$(14) \quad \operatorname*{Min}_{a_i} \operatorname*{Max}_{0 \leq x < \infty} \left| \frac{(-1)^n n!}{(1+x)^{n-1}} + \cdots + (-1)^{n-1} a_{n-1} \right| \Big/ |y|^n = \frac{n!}{2^{2n-1} |y|^n} \quad ,$$

which, if $\operatorname{Re}(y)$ is small, will be less than $n! / 2^{2n+1} |y|^n \operatorname{Re}(y)$.

§4. Application to the Error Function.

Referring to (6) of §1, it is sufficient to consider

$$(1) \quad g(y) = \int_0^\infty \frac{e^{-xy}}{(1+x)^{1/2}} \, dx \ .$$

In this case, we have the problem of determining

$$(2) \quad \operatorname*{Min}_{a_i} \operatorname*{Max}_{0 \leq x < \infty} \left| f^{(n)}(x) + a_1 f^{(n-1)}(x) + \cdots + a_n f(x) + a_{n+1} \right| \ ,$$

where $f(x) = (1+x)^{-1/2}$. Taking $a_{n+1} = 0$, we obtain as a bound

$$(3) \quad \operatorname*{Min}_{a_i} \operatorname*{Max}_{0 \leq x < \infty} \left| (1+x)^{-1/2} \left(\frac{(\frac{1}{2})(\frac{3}{2}) \cdots (\frac{2n-1}{2})}{(1+x)^n} + \cdots + a_n \right) \right|$$

$$\leq \operatorname*{Min}_{a_i} \operatorname*{Max}_{0 \leq x < \infty} \left| \frac{1 \cdot 3 \cdots (2n-1)}{2^n (1+x)^n} + \cdots + a_n \right|$$

$$= \frac{1 \cdot 3 \cdots (2n-1)}{2^n \, 2^{n-1}} \ .$$

Similarly, we can obtain bounds for the general integral

(4) $$I_a(y) = \int_0^\infty \frac{e^{-xy}}{(1+x)^a}\, dx \ ,$$

or integrals of the form

(5) $$J_a(y) = \int_0^\infty \frac{e^{-xy-x^n}}{(1-x)^a}\, dx \ .$$